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The program of the symposium was devoted to discussions of various theoretical methods which can be employed in studies of the atomic structures and atomic level phenomena associated with lattice defects such as grain boundaries, interfaces, dislocations, point defects and surfaces. The emphasis was on those approaches which can be used when developing a microscopic understanding of the properties of structural rather than electronic materials. The goal was to discuss methods based on the recent developments in the solid state physics in the framework of which the effect of the electronic structure can be directly taken into account. The papers presented at the symposium approached this goal on several different levels. On the semi-empirical level, where the input of the solid state theory is only indirect, the Embedded Atom Methos and Many body Potentials were discussed. A substantial part of the meeting was devoted to empirical approaches. Finally, the present status of the state of the art self-consistent abinitio calculations was reviewed. The symposium thus covered a wide range of newly developing approaches towards studies of the material behavior

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and served as a platform for a thorough discussion of both the merits and drawbacks of different approaches. The symposium thus certainly achieved its goal.

Report on the Symposium on

ATOMISTIC MODELING OF MATERIALS: BEYOND PAIR POTENTIALS

held during the World Materials Congress at Chicago from 27th till 30th September 1988 which was partially supported by the Air Force Office of Scientific Research.

The program of the symposium was devoted to discussions of various theoretical methods which can be employed in studies of the atomic structures and atomic level phenomena associated with lattice defects such as grain boundaries, interfaces, dislocations,point defects and surfaces. The emphasis was on those approaches which which can be used when developing a microscopic understanding of the properties of structural rather than electronic materials. The goal was to discuss methods based on the recent developments in the solid state physics in the framework of which the effect of the electronic structure can be directly taken into account. The papers presented at the symposium approached this goal on several different levels. On the semi-empirical level, where the input of the solid state theory is only indirect, the Embedded Atom Method and Many Body Potentials were discussed. A substantial part of the meeting was devoted to tight-binding methods which represent an intermediate step between ab-initio and semi-empirical approaches. Finally, the present status of the state of the art self-consistent ab-initio calculations was reviewed. The symposium thus covered a wide range of newly developing approaches towards studies of the material behavior and served as a plat form for a thorough discussion of both the merits and drawbacks of different approaches. The symposium thus certainly achieved its goal.

A very important factor in attaining the task of the symposium was the presence of a number of leading experts not only from the USA but other countries (Great Britain, Germany, France, Japan, Sweden). Many of them were invited speakers. Both the importance of the subject and the presence of the leading experts in the field attracted a large number of submitted papers as well as a large audience during the symposium. On average between sixty and seventy people were attending the symposium sessions and the audience decreased only slightly even during the last day of the symposium.

The papers presented at the symposium will be published in the Proceedings which are being prepared at present. by the Plenum Press. It is expected that the publication will appear in May or June.

Enclosure: Copy of the Symposium Program.

10:00 a.m.: **Properties of Magnetic Epitaxial Multilayers:** M B Salamon, University of Illinois, Urbana, IL

10:30 a.m.: **Intermission**

10:45 a.m.: **Electronic Structure of Layered Structures and Intermetallic Compounds:** A J Freeman, Northwestern University, Evanston, IL

ABSRACT: A status report is given of current state of the art theoretical approaches to understanding the electronic structure and properties of layered structures and intermetallic compounds Examples includes superlattices, high temperature structural materials and high T_c superconductors

11:45 a.m.: ***Structure-Induced Modulus Effects in Layered Superlattices:*** J F Lutsko, D Wolf, Argonne National Laboratory, Argonne, IL

SESSION F

Wednesday, 28 September, 2:00 p.m.-5:00 p.m.

Room L-14, McCormick Place North

Session Co-Chairmen: D A Payne
University of Illinois
Urbana, IL

R B Poeppel
Argonne National Laboratory
Argonne, IL

2:00 p.m.: **Preparation and Characterization of Ceramic Powder:** H K Bowen, M J Cima, Massachusetts Institute of Technology, Cambridge, MA

ABSTRACT: The development of chemical methods for the production of ceramic powders with controlled morphology has revealed the importance on unagglomerated, submicron, narrow-size distribution powders for manufacturing of ceramic devices These methods have been successfully applied to as variety of ceramic materials composed of a single cation Recent interest has, however, focused on chemical techniques to produce monosized powders of complex composition (compounds, alloys, and composite powders) Such powders could improve performance and reliability while simultaneously meeting the economic requirements of an increasingly competitive market Conventional methods will be reviewed for the preparation of complex oxides as well as advanced chemical techniques such as cohydrolysis of multicomponent alkoxide solutions, coacervation, and the combination of sol-gel and emulsion methods for the control of powder morphology and crystallinity Colloidal preparation methods for powder production have renewed interest in the hydrothermal conversion of the typically amorphous powder produced by most chemical methods to an unagglomerated, crystalline material Processes using hydrothermal reactions may be envisioned that proceed from the particle-synthesis stage to the finished greenbody without intermediate drying of the powder Techniques will be reviewed that have been used for the characterization of ceramic precursors and powder at different stages of processing

3:00 p.m.: Intermission

3:15 p.m.: **Consolidation of Ceramics:** D L Johnson, Northwestern University, Evanston, IL

ABSTRACT: The properties of modern ceramics depend critically upon the densities and grain sizes that can be achieved during the firing process Often properties are the most favorably influenced by obtaining the least porosity and the smallest grain size possible A number of techniques have been developed to achieve these, including careful powder processing to control the green microstructure, doping, pressure augmented consolidation such as uniaxial and isostatic hot pressing and sinter-forging, and fast firing employing conventional as well as plasma and microwave heating Sintering theory provides insight into the effects of applied pressure and high heating rates on sintering

4:15 p.m.: **Computer Simulation of Late Stage Singering:** D J Srolovitz, University of Michigan, Ann Arbor, MI

4:45 p.m.: **Microstructural Evolution in Silicon Nitride at Elevated Temperatures:** M Chadwick, T Malis, D S Wilkinson, CANMET, Ottawa, Ontario, Canada

SESSION G

Thursday, 29 September, 9:00 a.m.-12:00 noon

Room L-14, McCormick Place North

Session Co-Chairmen: M V Nevitt
Argonne National Laboratory
Argonne, IL

T O Mason
Northwestern University
Evanston, IL

9:00 a.m.: **Application of Phase Transformation in New Ceramics:** M Ruhle, University of California, Santa Barbara, CA

ABSTRACT: A comprehensive review of different toughening mechanisms in transformable brittle solids will be presented Emphasis is given to transformation toughening and microcrack toughening, although deflection toughening and toughening by second phases are also considered Existing models and theories are developed using concepts form applied mechanics but within the frame of thermodynamics and kinetics of the transformation process The theoretical results are compared with experimental data for various ZrO_2 containing ceramic alloys The dependency of the toughness on microstructural data will be discussed It is concluded that the toughening mechanism depends on the alloy composition and microstructure. Dilatational transformation toughening (with shear modifications) dominates in partially stabilized zirconia, different mechanisms may be included for other zirconia containing ceramics.

10:00 a.m.: **Theory of Phase Transformation in Ceramics:** S K Chan, Argonne National Laboratory, Argonne, IL

10:30 a.m.: **Intermission**

10:45 a.m.: **Electronic Ceramics:** R E Newnham, Pennsylvania State University, University Park, PA

ABSTRACT: Rapid progress in the integration and miniaturization of ceramic components has led to the development of multipurpose electronic packages containing complex three-dimensional circuitry At the same time a wide variety of smart sensors, transducers, and actuators are being constructed utilizing composite materials to concentrate fields and forces At present the processing methods make use of tape casting and thick film techniques, but a number of upset technologies loom on the horizon. During the years ahead we can expect electroceramic devices to follow in the footsteps of semiconductor technology as the component sizes drop below 1 micron, and nanocomposite devices and optoelectronic systems become a reality

11:45 a.m.: **Effects of Substitution on Superconducting Transition in $YBa_2Cu_3O_{7-\sigma}$:** B W Veal, Argonne National Laboratory, Argonne, IL

ATOMISTIC MODELING OF MATERIALS: BEYOND PAIR POTENTIALS

Sponsored by the Computer Simulation Committee of the Materials Science Division of ASM INTERNATIONAL

Program Co-Organizers: D J Srolovitz
University of Michigan
Ann Arbor, MI

V Vitek
University of Pennsylvania
Philadelphia, PA

SESSION I

Tuesday, 27 September, 9:00 a.m.-12:00 noon

Room L-15, McCormick Place North

Session Chairman: V Vitek
University of Pennsylvania
Philadelphia, PA

9:00 a.m.: **Electronic Structure, Total Energy and Force Calculations for Ordered and Disordered Materials with the LMTO Method:** O K Anderson, Max-Planck Institut fur Festkorperforschung, Stuttgart, Germany

ABSTRACT: Linear muffin-tin orbitals (LMTOs) constitute a minimal basis well suited for density functional calculations for complex systems containing s-, p-, d-, or f-electrons New Full-Potential LMTO techniques yield accurate total energies for impurity - and interface geometries and amphorous systems.

9:25 a.m.: **Multibody Potentials from Ab Initio Electronic Structure Calculations:** W A Goddard, III, California Institute of Technology, Pasadena, CA

ABSTRACT: From ab initio electronic structure calculations on clusters of atoms, it is possible to obtain multibody potentials that are useful in simulating materials. Strategies for obtaining transferable potentials from such calculations are discussed

9:50 a.m.: **Configurational Interactions in Binary Alloys:** A Gonis, P E A Turchi, Lawrence Livermore National Laboratory, Livermore, CA; G M Stocks, D M Nicholson, Oak Ridge National Laboratory, Oak Ridge, TN; X-G Zhang, Northwestern University, Evanston, IL

ABSTRACT: Three approaches to the calculation of effective pair and multisite interactions in binary alloys, the method of concentration waves, the generalized perturbation method and the embedded cluster method are discussed and compared.

10:15 a.m.: **Simulation of Isoelectronic Impurities in MgO Using Hartree-Fock Clusters:** J Zuo, R Pandey, A B Kunz, Michigan Technological University, Houghton, MI

10:40 a.m.: **Local Density Calculations of Defect Abundances and Diffusion Mechanics in Diamond, SiC, Si and Ge:** J Bernholc, A Antonelli, C Wang, R F Davis, North Carolina State University, Raleigh, NC; S T Pantelides, IBM Watson Research Division, Yorktown Heights, NY

ABSTRACT: This talk will review the recent advances in our understanding of the formation and diffusion in group IV semiconductors It will focus on self-diffusion mechanisms in diamond and Si, and on the effects of stoichiometry and Fermi level position on the relative abundance of native defects of cubic SiC.

11:05 a.m.: ***Microscopic Theory of Zone Folding Effects in Semiconductor Superlattices:*** M Jaros, K B Wong, P J Hagon, I Morrison, A Zoryk, L D L Brown, University of Newcastle, Newcastle-upon-Tyne, England

11:30 a.m.: **Total Energy Band Theory with the Fixed-Spin-Moment Procedure and Magnetic Properties of the Transition Elements:** P M Marcus, V L Moruzzi, IBM Research Division, T J Watson Research Center, Yorktown Heights, NY

SESSION II

Tuesday, 27 September, 2:00 p.m.-5:00 p.m.

Room L-15, McCormick Place North

Session Chairman: D G Pettifor
Imperial College of Science and Technology
London, England

2:00 p.m.: **Structural, Electron, Magnetic and Mechanical Properties of Materials via a Total Energy All-Electron Theory:** A J Freeman, Northwestern University, Evanston, IL

ABSTRACT: State-of-the art theoretical calculations of various properties of materials now accessible with a highly precise all-electron total-energy local density approach are reviewed. Examples include complex bulk solids (intermetallic compounds, high T_c superconducting oxides) and artificial materials (metal and semiconductor super-lattices and surfaces and interfaces).

2:25 p.m.: **Theory of Defects in Solids and Their Interactions:** A.B. Kunz, Michigan Technological University, Houghton, MI

ABSTRACT: Many-body theory of molecules is extended to include the interaction of an ensemble of atoms with an environment to simulate the properties of defects in the solid. The possibilities of using such a theory will be illustrated by several specific examples on the areas of oxides and ceramic materials.

2:50 p.m.: **From the Finite to the Infinite: The Structure of Clusters and Solids:** J.R. Chelikowsky, University of Minnesota, Minneapolis, MN

ABSTRACT: One of the most difficult condensed matter regimens to describe structurally is that of a large, finite system. Some solid state methods, based on pseudopotentials and local bases, for predicting the structural properties of both crystals and clusters, are reviewed. General approaches for large systems are applied to semiconductor clusters

3:15 p.m.: **MnTe and Spin Dependent Local-Density Theory: The Relation Between Spin- Polarized Conduction Bands and the Antiferromagnetic Ground State:** J.D. Dow, University of Notre Dame, Notre Dame, IN

ABSTRACT: Calculations using the spin-unrestricted pseudo-function method reveal that the s and p valence electrons on Mn atoms in anti-ferromagnetic zinc-blende MnTe are spin polarized in the ground state, as the d electrons are. This Hund's rule spin configuration enhances superexchange interactions. The resulted d-band positions agree well the photoemission data.

3:40 p.m.: **Applications of Simulated Annealing in Electronic Structure Studies of Metallic Clusters:** M.R. Pederson, Naval Research Lab., Washington, DC; J.Q. Broughton, State University of New York, Stony Brook, NY

ABSTRACT: A Gaussian based computational scheme for studies of isolated clusters is discussed. We have employed Car-Parrinello-like algorithms as well as conjugate gradient techniques to optimize the linear wavefunction expansion parameters as well as the non-linear Gaussian positions, accurate energy derivations are obtained. Applications to lithium clusters will be presented.

4:05 p.m.: **Ab-Initio Molecular Dynamics Simulation of Alkali Metal Microclusters:** W. Andreoni, IBM Research Division, Zurich, Switzerland; P. Ballone, Cornell University, Ithaca, NY; R. Carr, M. Parrinello, International School of Advanced Studies, Trieste, Italy

ABSTRACT: We perform a molecular dynamics simulation of alkali metal microclusters Na_N, K_N, Na_{N-X}, K_X, N up to 20). Total energy and interionic forces are computed for DFT in the LDA approximations. MD is used to perform a simulated annealing search for the ground state and to investigate thermal properties of the these systems.

4:30 p.m.: **A Simplified First Principles Tight-Binding-like Method for Electronic-Structure Based Molecular Dynamics Simulation:** O.F. Sankey, D. Niklewski, Arizona State University, Tempe, AZ

SESSION III
Wednesday, 28 September, 9:00 a.m.-12:00 noon
Room L-15, McCormick Place North
Session Chairman: A.J. Freeman
Northwestern University
Evanston, IL

9:00 a.m. **Multi-Atom Forces in Transition Metals and Semiconductors:** A.E. Carlsson, Washington University, St. Louis, MO

ABSTRACT: For accurate atomistic treatments of materials properties, it is necessary to include multi-atom forces. Several recent approaches for deriving such forces will be described and reviewed. Angle-dependent forces have been developed which explicitly take into account the shape of the electronic density of states.

9:25 a.m.: **First Principal Pseudopotential Studies of Cohesion in 3D Transition Metals:** E.J. Mele, M.-H. Kang, I. Morrison, University of Pennsylvania, Philadelphia, PA

ABSTRACT: A real space formulation of the mixed basis pseudopotential method is used to examine the ground state structural properties of several bulk and surface systems containing elements from the 3d transition series. Results are presented for Cu in a bct crystal system.

9:50 a.m.: **Calculation of Ground- and Excited-State Properties of Solids, Surfaces and Interfaces:** S.G. Louie, University of California, Berkeley, CA

ABSTRACT: A number of methods exist for calculation of the structural and electronic properties of materials. A combined *ab initio* pseudopotential- local density functional method for structural energies and Green's function quasiparticle method for electronic excitation spectra is discussed.

10:15 a.m.: **Molecular Dynamics Simulation of the Physics of Thin Film Growth on Si: Effects of the Properties of Interatomic Potential Models:** W.L. Morgan, University of Colorado, Boulder, CO

ABSTRACT: The molecular dynamics simulation of silicon and gallium thin film growth on reconstructed silicon surfaces will be presented. Results that depend on the properties of the interatomic potentials used will be discussed.

10:40 a.m.: **Self-Consistent Cluster-Lattice Simulation of Impurities in Ionic Crystals:** J. Meng, A.B. Kunz, Michigan Technological University, Houghton, MI

ABSTRACT: Electronic structure including the ground state energy, excited state energy, crystal field splitting, and vibrational frequency are calculated for impurity ions in alkali halides based on embedded unrestricted Hartree-Fock clusters with correlation correction.

11:05 a.m.: **Effective Medium Approach to the Energetics of Icosahedral and Other Complex Alloy Phases:** A. Zangwill, A. Redfield, Georgia Institute of Technology, Atlanta, GA

11:30 a.m.: **Structural and Electronic Properties of Amorphous Carbon:** G. Galli, R.M. Martin, University of Illinois at Urbana-Champaign, Urbana, IL; R. Carr, M. Parrinello, International School of Advanced Studies, Trieste, Italy

SESSION IV
Wednesday, 28 September, 2:00 p.m.-5:20 p.m.
Room L-15, McCormick Place North
Session Chairman: P.J. Hay
Los Alamos National Laboratory
Los Alamos, NM

2:00 p.m.: **Computer Modelling of Crystals and Glasses Using Many-Body Potentials:** C.R.A. Catlow, University of Keele, Staffordshire, England

ABSTRACT: Recent developments in the inclusion of many-body terms in potentials for polar materials are reviewed. Two types of formalism will be described: the use of bond-angle, harmonic functions and the use of triple dipole terms.

2:20 p.m.: **Embedded Atom Method: Many-Body Description of Metallic Cohesion:** M.S. Daw, Sandia National Laboratories, Livermore, CA

ABSTRACT: The Embedded Atom Method (EAM) is a new method for atomistic simulations of metals. The EAM is an efficient form that consumes no more computer time than 2-body interactions, but includes many-body effects important in metallic cohesion.

2:40 p.m.: **Many-Body Potentials for Disordered and Ordered Cubic Alloys:** G.J. Ackland, V. Vitek, University of Pennsylvania, Philadelphia, PA

ABSTRACT: Using a formalism analogous to that proposed by Finnis and Sinclair for transition metals, we derived model many-body potentials for noble metal alloy systems. The most important extension of the model is a simple incorporation of interspecies interactions. The observed phenomena of ordered Cu-Au alloys, disordered Au-Ag alloys and a segregated Cu-Ag system were all well reproduced in this scheme. The similarity of our results to those obtained by more complex electronic calculations leads us to suggest that details of electronic structure may be less important in determining atomic structures than are the more global effects such as atomic sizes and binding energies.

3:00 p.m.: **Many-Body Potentials for Hexagonal-Close-Packed Metals:** M. Igarashi, M. Khantha, V. Vitek, University of Pennsylvania, Philadelphia, PA

ABSTRACT: Many-body potentials of the Finnis-Sinclair type have been constructed for Mg, Co, Ti, Zr and Hf. Each potential ensures the stability of the non-ideal h.c.p. lattice with respect to any f.c.c. or b.c.c. lattice and any large deformation, and corresponding stacking-fault energies have reasonable values. Phonon-dispersion relations were also calculated.

3:20 p.m.: **Derivation of Embedding Functions to Reproduce Elastic and Vibrational Qualities of BCC Metals:** J.M. Eridon, Naval Research Laboratory, Washington, DC; S. Rao, Virginia Polytechnic and State University, Blacksburg, VA

ABSTRACT: A method has been developed to derive pair potentials, "electron densities," and embedding functions for bcc metals in such a way that the resulting model exactly reproduces long-wavelength (elastic constants) and short wavelength (zone boundary frequency) parameters of bcc metals. The application to iron and niobium will be discussed.

3:40 p.m.: **An Embedded Atom Potential for Iron:** R.J. Harrison, U.S. Army Materials Technology Laboratory, Watertown, MA; A.F. Voter, S.P. Chen, Los Alamos National Laboratory, Los Alamos, NM

ABSTRACT: An embedded atom potential for iron has been constructed which, like other EAM potentials, is fit exactly to bulk modulus, lattice parameter and sublimation energy. Individual elastic constants show deviations of about 20%. A constraint maintained in developing the potential was that the bcc energy be lower than fcc or hcp. Applications of the potential include simulations of surfaces and grain boundaries.

4:00 p.m.: **Effects of Boron and Sulfur on Ni_3Al Grain Boundaries:** A.F. Voter, S.P. Chen, R.C. Albers, A.M. Boring, P.J. Hay, Los Alamos National Laboratory, Los Alamos, NM

ABSTRACT: We have applied the embedded atom method to Ni_3Al grain boundaries with segregated B and S. The B and S potentials were fit almost exclusively to properties calculated using electronic band structure methods. Details of the fitting procedure will be presented, along with the effects of B and S on the boundary cohesive properties.

4:20 p.m.: **Embedded Atom Method Model for Close-Packed Metals:** D.J. Oh, R.A. Johnson, University of Virginia, Charlottesville, VA

ABSTRACT: A simple Embedded Atom potential for close-packed metals has been developed. Both the electron density function and the two-body potential are approximated by exponentially decreasing terms with a smooth cutoff. The embedding function contains terms linear and to an adjustable power of the electron density. The model has been applied successfully to five FCC metals and four HCP metals.

4:40 p.m.: **Boundary Conditions for Quantum Clusters Embedded in Classical Ionic Crystals:** J.M. Vail, University of Manitoba, Winnipeg, Canada

ABSTRACT: The ion-size effect is described for an embedded quantum cluster, and its representation by Kunz-Klein localizing potentials is described. Calculated results are given for perfect-lattice clusters, F centers and impurities. Features discussed include interionic forces, charge transfer, lattice distortion, and defect localization.

5:00 p.m.: **Impurity Effects on Grain Boundaries in Ni_3Al:** A.F. Voter, S.P. Chen, R.C. Albers, A.M. Boring, P.J. Hay, Los Alamos National Laboratories, Los Alamos, NM

SESSION V

Thursday, 29 September, 9:00 a.m.-12:00 noon
Room L-15, McCormick Place North

Session Chairman: J.J. Eberhardt
U.S. Department of Energy
Washington, DC

9:00 a.m.: **Physical Properties of Grain Boundaries from EAM Potentials:** D. Wolf, J.F. Lutsko, Argonne National Laboratory, Argonne, IL

ABSTRACT: One of the most pronounced structural features of grain boundaries lies in the local volume expansion due to the destruction of the perfect- crystal stacking at the interface. EAM potentials were used to investigate this volume expansion and its effect on thermodynamic properties and elastic constants.

9:25 a.m.: **Temperature Dependence of Interatomic Forces:** A.P. Sutton, Oxford University, Oxford, England

ABSTRACT: The temperature dependence of interatomic force in a three-dimensional solid is studied. The time averaged atomic structure of a solid at elevated temperature may be deduced with an energy minimization code (molecular statics).

9:50 a.m.: **Defect Energies via Equivalent Crystals:** J.R. Smith, General Motors Research Laboratories, Warren, MI; A. Banerjea, NASA Lewis Research Center, Cleveland, OH

ABSTRACT: Total energies are computed as if each atom were in a crystalline environment, with the crystal lattice constant chosen so that the total energy is equal to that of the defect solid. Example applications will be discussed, including the computation of surface properties of a variety of transitional metals.

10:15 a.m.: **Thermodynamics of Silicon Grain Boundaries from Zero Temperature to Melting:** S.R. Philpot, J.F. Lutsko, D. Wolf, Argonne National Laboratory, Argonne, IL

10:40 a.m.: **An Empirical Potential for Carbon, Its Polymorphs and Their Defects:** J. Tersoff, IBM Watson Research Center, Yorktown Heights, NY

ABSTRACT: A new empirical potential for carbon is described. It reproduces elastic constants, phonon energies, and defect energies in diamond and graphite rather well, opening a new range of materials for atomistic simulation. Simulations of amorphous carbon formation by quenching of the liquid have also been performed.

11:05 a.m.: **Energetics and Dynamics of Intrinsic Defects in Quenched Amorphous Silicon:** P.C. Kelires, J. Tersoff, IBM Watson Research Center, Yorktown Heights, NY

ABSTRACT: Properties of native defects in quenched amorphous silicon are studied using simulations with the empirical interatomic potentials of Tersoff and Stillinger-Weber. We infer the freeze-in temperature and formation energies of 3- and 5-fold coordinated defect atoms. We have also studied the spatial distribution of these defects and their interactions during annealing.

11:30 a.m.: **An Interatomic Potential Description of Local Icosahedral Packing in Transition Metal Systems: R.B. Phillips, A.E. Carlsson, Washington University, St. Louis, MO**

ABSTRACT: New interatomic potentials based on the moments of the electronic density of states have been developed within the framework of a d-band tight binding model. These potentials facilitate a local description of the bonding in phases with local icosahedral packing. Comparison of configurations in icosahedral phases and in the fcc structure shows that the energy penalty paid for 4-atom square clusters distinguishes the fcc energetics from icosahedral structures.

SESSION VI

Thursday, 29 September, 2:00 p.m.-5:00 p.m.
Room L-15, McCormick Place North

Session Chairman: O.K. Anderson
Max-Planck Institut fur Festkorperforschung
Stuttgart, West Germany

2:00 p.m.: **Tight-Binding Approach to the Total-Energy of Solids:** D.J. Chadi, Xerox Palo Alto Research Center, Palo Alto, CA

ABSTRACT: The semi-empirical tight-binding method has been developed during the last decade into a powerful and convenient tool in total-energy studies. Recent developments and limitations are discussed. In this talk the ideas underlying the method are reviewed and the results of a number of applications are examined.

2:25 p.m.: **The Tight-Binding Bond Model:** D.G. Pettifor, Imperial College of Science and Technology, London, England

ABSTRACT: A successful qualititative scheme for predicting structural trends and cohesive properties of materials is the Tight Binding model. It can be justified within the density functional theory starting from Harris' recent ideas.

2:50 p.m.: **Interatomic Forces in Silicon in the Tight-Binding Approximation: Structural Stability and Grain Boundary Structure:** A.T. Paxton, Max-Planck Institut fur Festkorperforschung, Stuttgart, Germany; A.P. Sutton, Oxford University, Oxford, England

ABSTRACT: A scheme is described for calculating interatomic forces in Si based on the semiempirical tight-binding bond model. Energy-volume curves demonstrate structural stability and relate the high-pressure phase transformation to changes in bond energies and s-p rehybridization.

3:15 p.m.: **Interatomic Potentials for Non-Metals Inferred from Ab Initio Calculations on Molecular Fragments:** M. Heggie, University of Exeter, Exeter, England

ABSTRACT: A new interatomic potential is presented that is based on the Wigner- Seitz cell characterizing each atom's local environment. The potential is intended to interpolate between results of local density pseudopotential calculations or distorted molecular fragments. Silicon Sp_2 and Sp_3 banding configurations are discussed.

3:40 p.m.: **Tight-Binding Models Direct from Density Functional Theory:** W.M. Foulkes, Cavendish Laboratory, Cambridge University, Cambridge, England

ABSTRACT: The expression for the total energy in semi-empirical tight-binding theory is shown to give a stationary estimate of the self-consistent ground state energy within density functional theory. Some successful applications, in which all the matrix elements and interatomic potentials were calculated without any adjustable parameters, are described.

4:05 p.m.: **LMTO Based Tight-Binding Method with Warping Correction for the Study of Defects in Transition and Noble Metals:** Y. Oh, V. Vitek, University of Pennsylvania, Philadelphia, PA

ABSTRACT: A parameterized TB method has been developed using first principle TB-LMTO-ASA. s, p and d electrons are treated in the same way and on-site elements are self-consistently related to off-site elements which are transferable. A warping correction has been added to account for effects of local straining which cannot be included in ASA.

4:30 p.m.: **Stability of the (110) Face in FCC Transition and Noble Metals Analyzed within a Tight-Binding Molecular Dynamics Scheme:** M. Guillope, B. Legrand, S.R.M.P.—CEN Saclay, Gif-sur-Yvette, France

ABSTRACT: 1. The stability of ther (110) surface structure is studied for the noble details within a simple tight-binding scheme. It is shown that the stable structure is the ideal one for Au and Ag anf the (1x2) russing row structure for Au. Moreover a (1x1) disordered structure is the stable one for all the noble metals at medium.

SESSION VII

Friday, 30 September, 9:00 a.m.-12:00 noon
Room L-15, McCormick Place North

Session Chairman: D.J. Srolovitz
University of Michigan
Ann Arbor, MI

9:00 a.m.: **Application of the Tight-Binding Bond Model:** M.W. Finnis, United Kingdom Atomic Energy Authority, Oxfordshire, England

ABSTRACT: Tight-Binding Bond model is a real space description of the energetics of materials, intermediate in realism between the classical pairwise force models and full self-consistent electron density functional theory. It is a variant of tight-binding, expressing energy and interatomic forces in terms of chemical bond orders and intersite matrix elements.

9:20 p.m.: **Beyond Pair-Potentials by Recursion Method:** R. Haydock, University of Oregon, Eugene, OR

ABSTRACT: In solids with extended defects, band structure methods of calculating electronic structure are limited to simple geometries. For complicated geometries, the recursion method can be applied not only to tight- binding and chemical pseudopotential electronic models, but to gaussian orbitals with gaussian pseudopotentials.

9:40 a.m.: **Application of Tight Binding Recursion Methods to Lattice Defects in Metals and Alloys:** K. Masuda-Jindo, Tokyo Institute of Technology, Yokohama, Japan; K. Kimura, S. Takeuchi, K. Tarakura, University of Tokyo, Tokyo, Japan

10:00 a.m.: **Atomistic Simulation of Superdislocation Dissociation in Ni_3Al:** M.H. Yoo, Oak Ridge National Laboratory, Oak Ridge, TN; M.S. Daw, M.I. Baskes, Sandia National Laboratory, Livermore, CA

10:20 a.m.: **Many-Atom Potentials for Intermetallic Compounds Obtained by Filtering the Results of Ab Initio Total Energy Calculations:** D.O. Welch, J.W. Davenport, Brookhaven National Laboratory, Upton, NY; R.D. Hatcher, City University of New York, Flushing, NY; M. Goldman, University of Pennsylvania, Philadelphia, PA

ABSTRACT: Semiempirical many-atom potentials were used to fit total energies from *ab initio* calculations for several simple hypothetical compounds of Nb and Sn, these potentials were used to compute properties of actual intermetallic compounds such as A15 and sigma phases.

10:40 a.m.: **A New Method for Coupled Elastic Atomistic Modeling:** S. Kohlhoff, Max-Planck- Institut fur Metallforschung, Stuttgart, Germany

ABSTRACT: A new method for elastic-atomistic coupled modeling is presented. It allows a more realistic treatment of the boundary conditions for atomistic simulations than previously possible. The method combines discrete atomistic description with a surrounding finite-element continuum. The analysis of an atomistically sharp crack is presented as an example.

11:00 a.m.: Atomistic Modeling of Diffusion Mechanisms of Impurities in Transition Metals Using the Embedded Atom Method: J.B. Adams, W.G. Wolfer, S.M. Foiles, Sandia National Laboratories, Livermore, CA

ABSTRACT: The self-diffusion and impurity diffusion of Cu, Ag, Au, Ni, Pd, and Pt have been calculated using the Embedded Atom Method (EAM). The diffusion rate of helium in nickel has been determined for four diffusion mechanisms (interstitial, dissociative, vacancy, exchange). These calculations are in reasonable agreement with experimental data.

SESSION VIII
Friday, 30 September, 2:00 p.m.-5:00 p.m.
Room L-15, McCormick Place North
Session Chairman: A.F. Voter
Los Alamos National Laboratory
Los Alamos, NM

2:00 p.m.: Simulations of Atomic Processes at Semiconductor Surfaces: R.E. Allen, Texas A&M University, College Station, TX

ABSTRACT: Many phenomena involving real materials are too complex for theoretical approaches. Computer simulation was used to predict the initial stages of atom-surface or molecule-surface interactions, including the chemisorption process, chemical trends in chemisorption, and the existence of initial chemisorption sites for a single species, etc.

2:20 p.m.: Interfaces, Structure, Growth, and Order in Tetrahedrally Bonded Materials: U. Landman, Georgia Institute of Technology, Atlanta, GA

ABSTRACT: Description of tetrahedrally bonded materials requires use of interaction potentials including non-additive three-body interactions. The topological characteristics, energetics and dynamics of amorphous silicon prepared via liquid quenching and alternatively by simulations of molecular-beam epitaxy (exhibiting tubular growth) are discussed.

2:40 p.m.: The Interaction of Cu, Pd, and Al with the GaAs (110) Surface: Metal-Ga Bonds and Schottky Barriers: R.W. Kasowski, E.I. DuPont, Wilmington, DE

3:00 p.m.: Semiconductor Surface Relaxation and Reconstruction Evaluated Using the Pseudo- Function Method: M.H. Tsai, University of Notre Dame, Notre Dame, IN

ABSTRACT: We have studied the zinc-blende (110) surface of eleven covalent and ionic compounds and wurtzite (10-10) surface of two relatively ionic compounds. The results show that relaxation/reconstruction of these surfaces is determined by a competition between covalent forces and Coulombic (ionic) forces. A dependence of the surface relaxation on ionicity is predicted.

3:20 p.m.: Oxidation of the GaAs (110) Surface: Comparison with Scanning Tunneling Microscope and Photoemission Data: W.E. Packard, University of Notre Dame, Notre Dame, IN

ABSTRACT: Using the pseudo-function method, our calculations for a selection of adsorption sites of a half-monolayer of oxygen on GaAs (110) show that oxygen atoms prefer to sit in the surface plane and to be multi-coordinated. The next preference is to bond to a single As surface atom. Comparison with low-coverage STM images will be given.

3:40 p.m.: Monte Carlo Simulation of Solute-Atom Segregation at Internal Interface Employing Embedded Atom Potentials for FCC Metals: M. Hwang, A. Seki, D.N. Seidman, A.J. Freeman, Northwestern University, Evanston, IL

4:00 p.m.: Molecular Dynamics Study of Grain Boundaries in Copper Segregated by Impurities of Bismuth and Silver: F.X. Zhou, Z.Y. Chen, Institute of Mechanics, Beijing, China; X.J. Wu, B. Hu, Academia Sinica, Hefei, China

4:20 p.m.: On Some Spectacular Results Concerning Surface Segregation in PtNi, AgNi, CuNi and ReRu Alloys Analyzed within a Tight-Binding Derived Ising Hamiltonian: B. Legrand, S.R.M.P.—CEN Saclay, Gif-sur-Yvette, France; G. Treglia, University Paris-Sud, Orsay, France

ABSTRACT: From the electronic structure of the disordered alloy we devise an effective Ising Hamiltonian for segregation and ordering processes at transition metal alloy surfaces. Using this tight-binding Ising Model (TBIM), we obtain spectacular results in PtNi, CuNi and AgNi alloys.

FOUR PERENNIAL TOPICS IN DEFORMATION: PAST, PRESENT AND FUTURE

Sponsored by the Flow and Fracture Committee of the Materials Science Division of ASM INTERNATIONAL
Program Organizers: R.J. Arsenault
University of Maryland
College Park, MD
B. MacDonald
National Science Foundation
Washington, DC

SESSION I: **Solid Solution Strengthening**
Monday, 26 September, 9:00 a.m.-12:00 noon
Room L-11, McCormick Place North
Session Co-Chairmen: B. MacDonald
National Science Foundation
Washington, DC
D. Hasson
U.S. Naval Academy
Annapolis, MD

9:00 a.m.: Solid Solution Strengthening: R.B. Schwarz, Los Alamos National Laboratory, Los Alamos, NM

9:45 a.m.: Review of Computer Simulation of Solid Solution Strengthening of FCC Alloys: R.J. Arsenault, University of Maryland, College Park, MD

ABSTRACT: Computer simulation techniques were used to explicate solid solution strengthening in fcc metals at 0°K. Thermally activated dislocation motion is a much more complicated process than that of dislocation motion of absolute zero temperature. Although there were no adjustable parameters in this study, agreement with experimental data was quite good.

10:30 a.m.: Solid Solution Strengthening: R.L. Fleischer, General Electric Research and Development Center, Schenectady, NY

ABSTRACT: Strengthening of crystals by elastic interaction with solute atoms or other atomic-sized defects is reviewed. One type of defects produce large lattice distortions, have a most tetragonal symmetry, and have first-order interaction with both screw and edge dislocations. Most substitutional atoms produce hardening from combined size and modulus effects.

11:15 a.m.: Mechanisms of Solution Hardening: H. Suzuki, Tokyo Engineering University, Tokyo, Japan

SESSION II: **High Temperature Creep**
Monday, 26 September, 2:00 p.m.-5:00 p.m.
Room L-11, McCormick Place North
Session Co-Chairmen: J.R. Weertman
Northwestern University
Evanston, IL
R.J. Arsenault
University of Maryland
College Park, MD

2:00 p.m.: Similitude and the Stress Exponent of Dislocation Power Law Creep: J. Weertman, Northwestern University, Evanston, IL

2:45 p.m.: The 0 Projection Concept—The Solution to a Perennial Problem: B. Wilshire, University College, Swansea, U.K.

3:30 p.m.: Creep of Intermetallic Compounds: D.P. Pope, University of Pennsylvania, Philadelphia, PA

ABSTRACT: There is currently a great deal of research being performed in many laboratories around the world on the mechanical properties of intermetallic compounds at high temperatures. In this paper, the work on creep deformation and creep fracture of these alloys will be reviewed, discussing first single phase, binary alloys having simple structures ($L1_2$, B2), then considering the more complex structures such as Do_{22}, A15, $L2_1$, etc. Finally, the results of current research on materials with relatively high melting temperatures, $T_m \geq 1500$ °C, will be discussed.

4:15 p.m.: Superplastic Behavior of Mechanically Alloyed Aluminum IN90211: A.K. Mukherjee, T.R. Bieler, University of California, Davis, CA; T.G. Nieh, J. Wadsworth, Lockheed Research Laboratory, Palo Alto, CA

SESSION III: **Work Hardening**
Tuesday, 27 September, 9:00 a.m.-12:00 noon
Room L-11, McCormick Place North
Session Co-Chairmen: H. Wilsdorf
University of Virginia
Charlottesville, VA
B. MacDonald
National Science Foundation
Washington, DC

9:00 a.m.: Work Hardening and Dynamical Recovery of FCC Metals in Multiple Glide: F.R.N. Nabarro, University of Witwatersrand, Johannesburg, South Africa

9:30 a.m.: Strain Hardening in FCC Polycrystals: U.F. Kocks, A.D. Rollett, Los Alamos National Laboratory, Los Alamos, NM

10:45 a.m.: Work-Hardening Through Low-Energy Dislocation Structures (LEDS): D. Kuhlmann-Wilsdorf, University of Virginia, Charlottesville, VA

ABSTRACT: The well-known, simple, very widely observed laws of work-hardening have long since been explained through the "Mesh-Length Theory" of work-hardening. It is shown that the few assumptions that had to be made in this theory result from the fact that dislocations form into LEDS, i.e., structures free of significant long-range stresses.

11:15 a.m.: Computational Modelling of Strain Hardening: R. Asaro, Brown University, Providence, RI

ABSTRACT: This talk is concerned with describing the transition of strain hardening on the microstructural level to macroscopic strain hardening behavior. On both levels the materials are taken to be strain rate dependent and subject to arbitrarily large strains. Examples are shown of full boundary value problems for metal single crystals, polycrystals, and polycrystalline composites. These are obtained by finite element computations. In these, the formation of shear bands is studied and the influence of shear bands on strain hardening.